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13. ABSTRACT (Maximum 200 words)  Algorithms, simulations and modeling for fluid mixing and complex flow were developed. Our front tracking algorithm was improved for its accuracy and conservation properties. Local mesh refinement was added. Simulations in agreement with experiment were obtained. New models of the fluid mixing process were derived, which were also compared to experimental data.					
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## A REPORT OUTLINE

1. ARO PROPOSAL NUMBER: 42254-MA
2. PERIOD COVERED BY REPORT: 15 June 2001 – 14 June 2004
3. TITLE OF PROPOSAL: Multiscale Modeling of Complex Physics: Fluids, Solids, Optics
4. CONTRACT OR GRANT NUMBER: DAAD19-01-1-0642
5. NAME OF INSTITUTION: State University of New York at Stony Brook
6. AUTHOR OF REPORT: James Glimm
7. APPENDICES, ILLUSTRATIONS, and TABLES: None
8. PROBLEM SOLVED:
  - Improved Front Tracking algorithms: Fully conservative, higher order accurate, automatic mesh refinement (AMR) and locally grid based resolution of interface bifurcations (for improved accuracy and robustness)
  - Simulations and theory for turbulent mixing rates in agreement with experimental data.

- Models for solution error for numerical simulation were developed and applied to engineering problems.
- Parallel FDTD photonics code with totally absorbing boundary conditions
- New algorithms for structural biology on ultra-fast parallel computers
- Technology Transfer to National Laboratories

9. SUMMARY OF MOST IMPORTANT RESULTS: See below.

10. TECHNOLOGY TRANSFER: Our photonics work is conducted as a collaboration with C. Bowden and M. Scalora of Redstone Arsenal. We interact with Tim Wright of ARL. J. Glimm has been chair of the External Advisory Board of the Weapons and Materials Science Directorate of ARL and a member of the Technical Advisory Board of ARL. He was also a member of the External Review Committee for the Dynamical Experimentation Division of Los Alamos National Laboratory.

The simulation code FronTier is in use at Los Alamos National Laboratory, both for fluid and for solid deformation modeling. It is used in fluid modeling in collaboration with staff of Livermore National Laboratory, Sandia National Laboratory and Brookhaven National Laboratory.

Work on photonics is in use for engineering design studies at Brookhaven National Laboratory.

Work on structural biology is in collaboration with crystallographers at Brookhaven National Laboratory.

Work on uncertainty quantification is in use at Los Alamos National Laboratory.

11. SCIENTIFIC PERSONNEL SUPPORTED BY THIS PROJECT AND DEGREES AWARDED WHILE EMPLOYED ON PROJECT:

- (a) Senior Personnel: Bradley Plohr
- (b) Post Docs: Yingjie Liu, Hyeonseong Jin, Erwin George
- (c) Graduate Students: Erwin George, Wei Guo, Jason Heller, Xinfeng Liu, Tianshi Lu, Jee-Yeon Nam, Shiqiang Wang, Yan Yu, Ming Zhao
- (d) Ph. D. Degrees Awarded (Students Supported by this Grant): Erwin George, Wei Guo, Jee-Yeon Nam

12. REPORT OF INVENTIONS (BY TITLE ONLY): No inventions were produced by the researchers.

13. COPIES OF TECHNICAL REPORTS: Sent Previously

**B LIST OF MANUSCRIPTS SUBMITTED OR PUBLISHED UNDER ARO SPONSORSHIP DURING THIS REPORTING PERIOD, INCLUDING JOURNAL REFERENCES**

## B.1 Peer Reviewed Publications

- [1] S. I. Abarzhi, J. Glimm, and An-Der Lin. Rayleigh-Taylor instability for fluids with a finite density contrast. *Phys. Fluids*, 15:2190–2197, 2003.
- [2] S. I. Abarzhi, J. Glimm, and K. Nishihara. Rayleigh-Taylor instability and Richtmyer-Meshkov instabilities for fluids with a finite density contrast. *Phys. Lett. A*, 11:1–7, 2003.
- [3] B. Cheng, J. Glimm, H. Jin, and D. H. Sharp. Theoretical methods for the determination of mixing. *Laser and Particle Beams*, 21:429–436, 2003.
- [4] B. Cheng, J. Glimm, and D. H. Sharp. Dynamical evolution of the Rayleigh-Taylor and Richtmyer-Meshkov mixing fronts. *Phys. Rev. E*, 66:1–7, 2002. Paper No. 036312.
- [5] B. Cheng, J. Glimm, and D. H. Sharp. Multi-temperature multiphase flow model. *ZAMP*, 53:211–238, 2002.
- [6] B. Cheng, J. Glimm, and D. H. Sharp. A three-dimensional renormalization group bubble merger model for Rayleigh-Taylor mixing. *Chaos*, 12:267–274, 2002.
- [7] Y. Deng, J. Glimm, J. Davenport, X. Cai, and E. Santos. Performance models on QCDOC for molecular dynamics with coulomb potentials. *International Journal of High Performance Computing Applications*, 18(SUNYSB-AMS-00-04):183–198, 2004.
- [8] B. DeVolder, J. Glimm, J. W. Grove, Y. Kang, Y. Lee, K. Pao, D. H. Sharp, and K. Ye. Uncertainty quantification for multiscale simulations. *Journal of Fluids Engineering*, 124:29–41, 2002. LANL report No. LA-UR-01-4022.
- [9] R. P. Drake, H. F. Robey, O. A. Hurricane, B. A. Remington, J. Knauer, J. Glimm, Y. Zhang, D. Arnett, D. D. Ryutov, J. O. Kane, K. S. Budil, and J. W. Grove. Experiments to produce a hydrodynamically unstable spherically diverging system of relevance to instabilities in supernovae. *Astrophysical Journal*, 564:896–906, 2002.
- [10] S. Dutta, E. George, J. Glimm, J. Grove, H. Jin, T. Lee, X. Li, D. H. Sharp, K. Ye, Y. Yu, Y. Zhang, and M. Zhao. Shock wave interactions in spherical and perturbed spherical geometries. Elsevier, 2004. University at Stony Brook preprint number SB-AMS-04-09 and LANL report No. LA-UR-04-2989.
- [11] E. George, J. Glimm, J. W. Grove, X. L. Li, Y. J. Liu, Z. L. Xu, and N. Zhao. Simplification, conservation and adaptivity in the front tracking method. In T. Hou and E. Tadmor, editors, *Hyperbolic Problems: Theory, Numerics, Applications*, pages 175–184. Springer Verlag, Berlin and New York, 2003.
- [12] E. George, J. Glimm, X. L. Li, A. Marchese, and Z. L. Xu. A comparison of experimental, theoretical, and numerical simulation Rayleigh-Taylor mixing rates. *Proc. National Academy of Sci.*, 99:2587–2592, 2002.

- [13] J. Glimm, J. W. Grove, Y. Kang, T. Lee, X. Li, D. H. Sharp, Y. Yu, K. Ye, and M. Zhao. Errors in numerical solutions of spherically symmetric shock physics problems. *Contemporary Mathematics*, 2004. University at Stony Brook Preprint Number SB-AMS-04-03, Los Alamos National Laboratory number LA-UR-04-0713.
- [14] J. Glimm, J. W. Grove, X. L. Li, W. Oh, and D. H. Sharp. A critical analysis of Rayleigh-Taylor growth rates. *J. Comp. Phys.*, 169:652–677, 2001.
- [15] J. Glimm, J. W. Grove, and Y. Zhang. Interface tracking for axisymmetric flows. *SIAM J. SciComp*, 24:208–236, 2002. LANL report No. LA-UR-01-448.
- [16] J. Glimm, J. W. Grove, Y. Zhang, and S. Dutta. Numerical study of axisymmetric Richtmyer-Meshkov instability and azimuthal effect on spherical mixing. *J. Stat. Physics*, 107:241–260, 2002.
- [17] J. Glimm, Yoon ha Lee, and Kenny Ye. A simple model for scale up error. *Contemporary Mathematics*, 295:241–251, 2002.
- [18] J. Glimm, S. Hou, H. Kim, Y. Lee, D. Sharp, K. Ye, and Q. Zou. Risk management for petroleum reservoir production: A simulation-based study of prediction. *J. Comp. Geosciences*, 5:173–197, 2001.
- [19] J. Glimm, S. Hou, Y. Lee, D. Sharp, and K. Ye. Solution error models for uncertainty quantification. *Contemporary Mathematics*, 327:115–140, 2003. SUNYSB preprint 02-16. LANL preprint LA-UR: 02-5987.
- [20] J. Glimm and H. Jin. An asymptotic analysis of two-phase fluid mixing. *Bol. Soc. Bras. Mat.*, 32:213–236, 2001.
- [21] J. Glimm, H. Jin, M. Laforest, F. Tangerman, and Y. Zhang. A two pressure numerical model of two fluid mixing. *SIAM J. Multiscale Model. Simul.*, 1:458–484, 2003.
- [22] J. Glimm, X.-L. Li, and A.-D. Lin. Nonuniform approach to terminal velocity for single mode Rayleigh-Taylor instability. *ACTA MATHEMATICAE APPLICATAE SINICA*, 18:1–8, 2002.
- [23] J. Glimm, X.-L. Li, and Y.-J. Liu. Conservative front tracking in higher space dimensions. *Transactions of Nanjing University of Aeronautics and Astronautics*, 18, Suppl.:1–15, 2001. Proceedings of International Workshop on Computational Methods for Continuum Physics and Their Applications (IWCCPA), Nanjing, China.
- [24] J. Glimm, X.-L. Li, and Y.-J. Liu. Conservative front tracking in one space dimension. *Contemporary Mathematics*, 295:253–264, 2002. Proceedings of the Joint Summer Research Conference on Fluid Flow and Transport in Porous Media: Mathematical and Numerical Treatment. In Press, Report SUNYSB-AMS-01-16.
- [25] J. Glimm, X.-L. Li, and Y.-J. Liu. Conservative front tracking with improved accuracy. *SIAM J. Numerical Analysis*, 41:1926–1947, 2003.

- [26] L. Li, J. Glimm, and X.-L. Li. All isomorphic distinct cases for multi-component interfaces in a block. *J. Comp. Appl. Mathematics*, 152:263–276, 2003.
- [27] N. Stojić, J. W. Davenport, M. Komelj, and J. Glimm. Surface magnetic moment in  $\alpha$ -uranium by density-functional theory. *Phys. Rev. B*, 68, 094407:(5 pages), 2003.
- [28] N. Stojic, J. Glimm, Y. Deng, and J. Haus. Transverse magnetic modes in two-dimensional triangular photonic crystals. *Phys. Rev. E*, 64:1–7, 2001. Paper number 056614.
- [29] Wei Zhu, Xuema Wang, Yeming Ma, Manlong Rao, James Glimm, and John Kovach. Detection of cancer specific markers amidst massive mass spectral data. *Proc. Nat. Aca. Sci.*, 100:14666–14671, 2003.

## B.2 Technical Reports

- [1] J. Glimm, J. W. Grove, Y. Kang, T. Lee, X. Li, D. H. Sharp, Y. Yu, K. Ye, and M. Zhao. Error analysis for shock interactions. Technical report, University at Stony Brook (Preprint number SB-AMS-03-14; LANL Preprint number LA-UR-03-6266), 2003.
- [2] J. Glimm, S. Hou, Y. Lee, D. Sharp, and K. Ye. Prediction of oil production with confidence intervals. SPE 66350, Society of Petroleum Engineers, 2001. SPE Reservoir Simulation Symposium held in Houston, Texas, 11-14 Feb.

### B.3 Submissions and Articles in Press

- [1] S. I. Abarzhi, J. Glimm, and An-Der Lin. Dynamics of the Rayleigh-Taylor bubbles for fluids with a finite density contrast. *Laser and Particle Beams*, 2003. accepted; Stony Brook University Preprint SUNYSB-AMS-02-11.
- [2] S. Dutta, E. George, J. Glimm, X. L. Li, A. Marchese, Z. L. Xu, Y. M. Zhang, J. W. Grove, and D. H. Sharp. Numerical methods for the determination of mixing. *Laser and Particle Beams*, 2003. accepted, LANL report No. LA-UR-02-1996.
- [3] S. Dutta, J. Glimm, J. W. Grove, D. H. Sharp, and Y. Zhang. Error comparison in tracked and untracked spherical simulations. *Computers and Mathematics with Applications*, 2003. accepted, University at Stony Brook preprint number AMS-03-10 and LANL report No. LA-UR-03-2920.
- [4] E. George and J. Glimm. Self similarity of Rayleigh-Taylor mixing rates. *Phys. Fluids*, 2004. Submitted. Stony Brook University Preprint number SUNYSB-AMS-04-05.
- [5] J. Glimm, J. W. Grove, Y. Kang, T. Lee, X. Li, D. H. Sharp, Y. Yu, K. Ye, and M. Zhao. Statistical riemann problems and a composition law for errors in numerical solutions of shock physics problems. *SISC (In Press)*, 2003. University at Stony Brook Preprint Number SB-AMS-03-11, Los Alamos National Laboratory number LA-UR-03-2921.
- [6] J. Glimm, S. Hou, Y. Lee, D. Sharp, and K. Ye. Sources of uncertainty and error in the simulation of flow in porous media. *Comp. and Applied Mathematics*, 2003. In Press. SUNYSB preprint 03-08. LANL preprint LA-UR-03-2328.
- [7] H. Jin, J. Glimm, and D. H. Sharp. Two-pressure two-phase flow models. *ZAMP*, 2003. Submitted. Stony Brook University Preprint number SUNYSB-AMS-03-16 and Los Alamos National Laboratory LAUR Number LA-UR-03-7279.
- [8] H. Jin, X. F. Liu, T. Lu, B. Cheng, J. Glimm, and D. H. Sharp. Rayleigh-Taylor mixing rates for compressible flow. *Phys. Fluids*, 2004. Submitted for publication. Stony Brook University Preprint number SUNYSB-AMS-04-06 and Los Alamos National Laboratory LAUR Number LA-04-1384.
- [9] R. Samulyak, J. Glimm, and W. Oh. A numerical algorithm for free MHD flows. *SISC (submitted)*, 2002. SUNY Stony Brook preprint.
- [10] J. Walter, D. Yu, B. J. Plohr, J. Grove, and J. Glimm. An algorithm for Eulerian front tracking for solid deformation. *SIAM J. Sci. Comput.*, 2003. to appear.
- [11] Y. Zhang, P. Drake, J. Glimm, J. Grove, and D. H. Sharp. Radiation coupled front tracking simulations for laser driven shock experiments. *J. Nonlinear Analysis*, 2004. Submitted. LANL report No. LA-UR-04-2381.

## B.4 Conference Proceedings

- [1] D. Brown, L. Freitag, and J. Glimm. Creating interoperable meshing and discretization software: The terascale simulation tools and technology center. In Bharat Soni, editor, *Proceedings of the 8th International Conference on Numerical Grid Generation in Computational Field Simulations, June 2-6, 2002, Honolulu Hawaii*. 2002.
- [2] B. Cheng, J. Glimm, X. L. Li, and D. H. Sharp. Subgrid models and DNS studies of fluid mixing. In E. Meshkov, Y. Yanilkin, and V. Zhmailo, editors, *Proceedings of the 7th International Conference on the Physics of Compressible Turbulent Mixing, (1999)*, pages 385–390, Sarov, Nizhny Novgorod region, Russia, 2001. RFNC-VNIIEF.
- [3] S. Dutta, J. Glimm, J. W. Grove, D. H. Sharp, and Y. Zhang. A fast algorithm for moving interface problems. In V. Kumar et al., editor, *Computational Science and Its Applications - ICCSA 2003, LNCS 2668*, pages 782–790. Springer-Verlag, Berlin Heidelberg, 2003. LANL report No. LA-UR-02-7895.
- [4] S. Dutta, J. Glimm, J. W. Grove, D. H. Sharp, and Y. Zhang. Spherical Richtmyer-Meshkov instability for axisymmetric flow. *Mathematics and Computers in Simulations*, 65:417–430, 2004. University at Stony Brook preprint number AMS-03-13.
- [5] J. Glimm, J. W. Grove, X. L. Li, Yingjie Liu, and Zhiliang Xu. Unstructured grids in 3D and 4D for time-dependent interface in front tracking with improved accuracy. In B. K. Soni et al., editor, *Proc. 8th Int. Conf. Num. Grid Generation in Comp. Field Simulations*, pages 179–188. 2002. LANL report No. LA-UR-02-0893.
- [6] J. Glimm, H. Jin, and Y. Zhang. Front tracking for multiphase fluid mixing. In A. A. Mammoli and C. A. Brebbia, editors, *Computational Methods in Multiphase Flow II*, pages 13–22. WIT Press, Southampton, UK, 2004.
- [7] J. Glimm, X.-L. Li, Y.-J. Liu, and N. Zhao. Conservative front tracking and level set algorithms. *Proc. National Academy of Sci.*, 98:14198–14201, 2001.
- [8] J. Glimm, X. L. Li, W. Oh, A. Marchese, M.-N. Kim, R. Samulyak, and C. Tzanos. Jet breakup and spray formation in a diesel engine. In *Proceedings of the Second MIT Conference on Computational Fluid and Solid Mechanics*. Cambridge, MA, 2003. SUNY Stony Brook preprint No. susb-ams-02-20.
- [9] James Glimm, Yunha Lee, David H Sharp, and Kenny Q Ye. Prediction using numerical simulations, A bayesian framework for uncertainty quantification and its statistical challenge. In Bilal M. Ayyub and Nii O. Attoh-Okine, editors, *Proceedings of the Fourth International Symposium on Uncertainty Modeling and Analysis (ISUMA 2003)*. IEEE, Computer Society, 2003.

- [10] T. Lee, Y. Yu, M. Zhao, J. Glimm, X. Li, and K. Ye. Error analysis of composite shock interaction problems. *Conference Proceedings of PMC04*, 2004. (submitted) University at Stony Brook Preprint Number SB-AMS-04-08.

## C SUMMARY OF MOST IMPORTANT RESULTS

**Introduction.** The principal thrust of our new simulations were fluid interface instabilities, solid dynamics, uncertainty quantification, structural biology and photonics. All of this work has joined developments in theory and modeling to our simulation results.

Additional Army-related activities of the project PI, James Glimm, within this reporting period include: chair of the External Advisory Board for the Weapons and Material Science Directorate of the ARL; a member of the Technical Advisory Board of ARL; member of the Technical Advisory Board of the Dynamic Testing Division of Los Alamos National Laboratory; and scientific interaction with Tim Wright of ARL and Chuck Bowden and Michale Scalora of Redstone Arsenal.

**Improved Front Tracking Algorithms** Four important improvements have been added to our Front Tracking simulations. These are:

- A capability for MHD has been added, with sharp boundaries between distinct MHD fluids having distinct conductivities.
- Automatic Mesh Refinement (AMR) has been added, through merger of our FronTier code with the LLNL Overture code. The AMR is patch based, and follows the Berger-Colella algorithm.
- Robust simple interface bifurcations have been achieved in 3D through use of a locally grid based interface description algorithm. Regions containing bifurcations have been reconstructed based on a reduced, grid related interface description. The algorithm is very robust. See [20, 47].
- Fully conservative front propagation has been achieved through a new tracking algorithm which tracks a discontinuity surface in space and time, [40, 39, 38, 41].

**Simulations and Theory for Turbulent Mixing** Definitive results have been obtained for the simulation [6, 26, 21, 15] of Rayleigh-Taylor flows, with the first agreement of simulation with experiment and theory [9, 5] for three dimensional acceleration driven (Rayleigh-Taylor) turbulent mixing. The importance of the agreement obtained by the FronTier simulations with experiment and theory is emphasized by the disagreement, by a factor of about two, between most codes and experiment for this problem. Instabilities in axisymmetric implosions and explosions were simulated [27, 28]. Validation studies and an exploration of the influence of axisymmetry in the problem definition on the statistics of the chaotic mixing were performed. Agreement with laser driven experiments [13] was obtained.

**Elastic-Plastic Flow.** Validation studies for the Front Tracking code FronTier-Solid have been performed [52]. Front Tracking is advantageous relative to traditional Lagrangian codes because the fixed Eulerian computational mesh is not subject to mesh distortion; it is advantageous relative to standard Eulerian codes because the tracking eliminates spurious numerical diffusion at interfaces and the need for artificial mixed-material computational cells. FronTier-Solid is a two-dimensional solid dynamics code based on a fully conservative formulation of the governing equations for large-strain deformation, a hyperelastic equation of state that allows for large volumetric change, and a rate-dependent plasticity model for

high strain rates. The code features conservative finite differencing, a Riemann solver that accounts for the nonlinearity of longitudinal waves, and an implicit method for integrating the plastic source term.

The Richtmyer-Meshkov shock driven instability was studied in elastic materials (i.e. with strength) in a Stony Brook Ph.D thesis [48]. The work focused on linearized solutions; it serves as a validation standard for nonlinear simulations. The unperturbed solution is obtained using the Riemann solver that is part of the FronTier Solid code. The corresponding linearized equations are solved numerically. The main result is a prediction of the growth rate of the perturbation amplitude.

**Uncertainty Quantification.** The purpose of this project is to assess and quantify the uncertainty of predictions made with simulation codes. As the codes are being used to make operational decisions, and as the degree of experimental testing is diminished, the verification and validation (V&V) of simulation codes becomes of increasing importance. Quantification of uncertainty may be viewed as an extension of whole V&V effort. It goes beyond asking the question, is the simulation correct, and more quantitatively, it asks, 'how correct is the simulation?', with a quantitative answer expressed in the form of error bars, confidence intervals, or some measure of uncertainty. In our earlier papers we found that the interplay between the forward and inverse problems, with Bayesian analysis to include the added information of experiments, was important. Also the study of probabilistic error models for numerical solution errors is important. Following this lead, we have begun a probabilistic study of solution errors [30, 31, 12], based on computer experiments to generate the numerical errors.

The point of view we have developed appears to be rather original, as we are not aware of comparable studies of numerical solution error. Most prior work on solution error assumed that the simulation is already fully resolved, and that the numerical solution is within the range of asymptotic convergence, so that theory based on numerical estimates of order of convergence can be applied. All of these assumptions are not likely to be valid for the simulation of complex problems.

**Photonics.** This is a new project, conducted in collaboration with C. Bowden and M. Scalora of Redstone Arsenal and their collaborators. We have developed a parallelized FDTD code with nonreflecting boundaries to allow simulations in complex 3D geometries for photonic crystals and other photonic devices [51]. We have built on our prior experience in parallel software development, and in construction of low cost parallel hardware.

Our program is specially designed to study finite photonic devices with three-dimensionally heterogeneous dielectrics. The changes in the dielectric function occur on the scale of the electromagnetic wavelength and the contrast between the dielectric constants is large. We consider applications to finite devices for frequency doublers and high quality cavities for VCSEL lasers. The code is being used to simulate application specific device geometries to resolve design issues. We are working with experimental groups to model the devices and optimize the parameter values.

We have conducted design studies for RF cavities and other accelerator components at Brookhaven National Laboratory using this code.

**Structural Biology on High Performance Hardware** We investigated [11, 10] the use of novel high performance hardware for structural biology (MD and MC) simulations.

The hardware target was a special purpose design, QCDOC, primarily intended for quantum gauge theory calculations. This machine is a precursor to the general purpose IBM machine BG/L, and both are unique in using a mesh rather than a switch for parallel communication. As a result, the machine has very attractive price performance behavior for large size (30K to 150K processor) configurations. We developed a simulation model of the force field calculation (especially for the Coulomb force), and project that it will be possible to simulate 100K atoms in an all atom simulation for up to 1 to 10  $\mu$  sec. We are developing an MD simulation code to run on QCDOC and in the meantime we are simulating Bolulinum, as a target molecule. This work is conducted in collaboration with crystallographers at Brookhaven National Laboratory.

## D BIBLIOGRAPHY

- [1] S. I. Abarzhi, J. Glimm, and An-Der Lin. Dynamics of the Rayleigh-Taylor bubbles for fluids with a finite density contrast. *Laser and Particle Beams*, 2003. accepted; Stony Brook University Preprint SUNYSB-AMS-02-11.
- [2] S. I. Abarzhi, J. Glimm, and An-Der Lin. Rayleigh-Taylor instability for fluids with a finite density contrast. *Phys. Fluids*, 15:2190–2197, 2003.
- [3] S. I. Abarzhi, J. Glimm, and K. Nishihara. Rayleigh-Taylor instability and Richtmyer-Meshkov instabilities for fluids with a finite density contrast. *Phys. Lett. A*, 11:1–7, 2003.
- [4] D. Brown, L. Freitag, and J. Glimm. Creating interoperable meshing and discretization software: The terascale simulation tools and technology center. In Bharat Soni, editor, *Proceedings of the 8th International Conference on Numerical Grid Generation in Computational Field Simulations, June 2-6, 2002, Honolulu Hawaii*. 2002.
- [5] B. Cheng, J. Glimm, H. Jin, and D. H. Sharp. Theoretical methods for the determination of mixing. *Laser and Particle Beams*, 21:429–436, 2003.
- [6] B. Cheng, J. Glimm, X. L. Li, and D. H. Sharp. Subgrid models and DNS studies of fluid mixing. In E. Meshkov, Y. Yanilkin, and V. Zhmailo, editors, *Proceedings of the 7th International Conference on the Physics of Compressible Turbulent Mixing, (1999)*, pages 385–390, Sarov, Nizhny Novgorod region, Russia, 2001. RFNC-VNIIEF.
- [7] B. Cheng, J. Glimm, and D. H. Sharp. Dynamical evolution of the Rayleigh-Taylor and Richtmyer-Meshkov mixing fronts. *Phys. Rev. E*, 66:1–7, 2002. Paper No. 036312.
- [8] B. Cheng, J. Glimm, and D. H. Sharp. Multi-temperature multiphase flow model. *ZAMP*, 53:211–238, 2002.

- [9] B. Cheng, J. Glimm, and D. H. Sharp. A three-dimensional renormalization group bubble merger model for Rayleigh-Taylor mixing. *Chaos*, 12:267–274, 2002.
- [10] J. Davenport, Y. Deng, and J. Glimm. Global communication schemes on QCDOC. *International Journal of High Performance Computing Applications*, 2003. Submitted.
- [11] Y. Deng, J. Glimm, J. Davenport, X. Cai, and E. Santos. Performance models on QCDOC for molecular dynamics with coulomb potentials. *International Journal of High Performance Computing Applications*, 18(SUNYSB-AMS-00-04):183–198, 2004.
- [12] B. DeVolder, J. Glimm, J. W. Grove, Y. Kang, Y. Lee, K. Pao, D. H. Sharp, and K. Ye. Uncertainty quantification for multiscale simulations. *Journal of Fluids Engineering*, 124:29–41, 2002. LANL report No. LA-UR-01-4022.
- [13] R. P. Drake, H. F. Robey, O. A. Hurricane, B. A. Remington, J. Knauer, J. Glimm, Y. Zhang, D. Arnett, D. D. Ryutov, J. O. Kane, K. S. Budil, and J. W. Grove. Experiments to produce a hydrodynamically unstable spherically diverging system of relevance to instabilities in supernovae. *Astrophysical Journal*, 564:896–906, 2002.
- [14] S. Dutta, E. George, J. Glimm, J. Grove, H. Jin, T. Lee, X. Li, D. H. Sharp, K. Ye, Y. Yu, Y. Zhang, and M. Zhao. Shock wave interactions in spherical and perturbed spherical geometries. Elsevier, 2004. University at Stony Brook preprint number SB-AMS-04-09 and LANL report No. LA-UR-04-2989.
- [15] S. Dutta, E. George, J. Glimm, X. L. Li, A. Marchese, Z. L. Xu, Y. M. Zhang, J. W. Grove, and D. H. Sharp. Numerical methods for the determination of mixing. *Laser and Particle Beams*, 2003. accepted, LANL report No. LA-UR-02-1996.
- [16] S. Dutta, J. Glimm, J. W. Grove, D. H. Sharp, and Y. Zhang. Error comparison in tracked and untracked spherical simulations. *Computers and Mathematics with Applications*, 2003. accepted, University at Stony Brook preprint number AMS-03-10 and LANL report No. LA-UR-03-2920.
- [17] S. Dutta, J. Glimm, J. W. Grove, D. H. Sharp, and Y. Zhang. A fast algorithm for moving interface problems. In V. Kumar et al., editor, *Computational Science and Its Applications - ICCSA 2003, LNCS 2668*, pages 782–790. Springer-Verlag, Berlin Heidelberg, 2003. LANL report No. LA-UR-02-7895.
- [18] S. Dutta, J. Glimm, J. W. Grove, D. H. Sharp, and Y. Zhang. Spherical Richtmyer-Meshkov instability for axisymmetric flow. *Mathematics and Computers in Simulations*, 65:417–430, 2004. University at Stony Brook preprint number AMS-03-13.
- [19] E. George and J. Glimm. Self similarity of Rayleigh-Taylor mixing rates. *Phys. Fluids*, 2004. Submitted. Stony Brook University Preprint number SUNYSB-AMS-04-05.
- [20] E. George, J. Glimm, J. W. Grove, X. L. Li, Y. J. Liu, Z. L. Xu, and N. Zhao. Simplification, conservation and adaptivity in the front tracking method. In T. Hou and E. Tadmor, editors, *Hyperbolic Problems: Theory, Numerics, Applications*, pages 175–184. Springer Verlag, Berlin and New York, 2003.

- [21] E. George, J. Glimm, X. L. Li, A. Marchese, and Z. L. Xu. A comparison of experimental, theoretical, and numerical simulation Rayleigh-Taylor mixing rates. *Proc. National Academy of Sci.*, 99:2587–2592, 2002.
- [22] J. Glimm, J. W. Grove, Y. Kang, T. Lee, X. Li, D. H. Sharp, Y. Yu, K. Ye, and M. Zhao. Error analysis for shock interactions. Technical report, University at Stony Brook (Preprint number SB-AMS-03-14; LANL Preprint number LA-UR-03-6266), 2003.
- [23] J. Glimm, J. W. Grove, Y. Kang, T. Lee, X. Li, D. H. Sharp, Y. Yu, K. Ye, and M. Zhao. Statistical riemann problems and a composition law for errors in numerical solutions of shock physics problems. *SISC (In Press)*, 2003. University at Stony Brook Preprint Number SB-AMS-03-11, Los Alamos National Laboratory number LA-UR-03-2921.
- [24] J. Glimm, J. W. Grove, Y. Kang, T. Lee, X. Li, D. H. Sharp, Y. Yu, K. Ye, and M. Zhao. Errors in numerical solutions of spherically symmetric shock physics problems. *Contemporary Mathematics*, 2004. University at Stony Brook Preprint Number SB-AMS-04-03, Los Alamos National Laboratory number LA-UR-04-0713.
- [25] J. Glimm, J. W. Grove, X. L. Li, Yingjie Liu, and Zhiliang Xu. Unstructured grids in 3D and 4D for time-dependent interface in front tracking with improved accuracy. In B. K. Soni et al., editor, *Proc. 8th Int. Conf. Num. Grid Generation in Comp. Field Simulations*, pages 179–188. 2002. LANL report No. LA-UR-02-0893.
- [26] J. Glimm, J. W. Grove, X. L. Li, W. Oh, and D. H. Sharp. A critical analysis of Rayleigh-Taylor growth rates. *J. Comp. Phys.*, 169:652–677, 2001.
- [27] J. Glimm, J. W. Grove, and Y. Zhang. Interface tracking for axisymmetric flows. *SIAM J. SciComp*, 24:208–236, 2002. LANL report No. LA-UR-01-448.
- [28] J. Glimm, J. W. Grove, Y. Zhang, and S. Dutta. Numerical study of axisymmetric Richtmyer-Meshkov instability and azimuthal effect on spherical mixing. *J. Stat. Physics*, 107:241–260, 2002.
- [29] J. Glimm, Yoon ha Lee, and Kenny Ye. A simple model for scale up error. *Contemporary Mathematics*, 295:241–251, 2002.
- [30] J. Glimm, S. Hou, H. Kim, Y. Lee, D. Sharp, K. Ye, and Q. Zou. Risk management for petroleum reservoir production: A simulation-based study of prediction. *J. Comp. Geosciences*, 5:173–197, 2001.
- [31] J. Glimm, S. Hou, Y. Lee, D. Sharp, and K. Ye. Prediction of oil production with confidence intervals. SPE 66350, Society of Petroleum Engineers, 2001. SPE Reservoir Simulation Symposium held in Houston, Texas, 11-14 Feb.
- [32] J. Glimm, S. Hou, Y. Lee, D. Sharp, and K. Ye. Solution error models for uncertainty quantification. *Contemporary Mathematics*, 327:115–140, 2003. SUNYSB preprint 02-16. LANL preprint LA-UR: 02-5987.

- [33] J. Glimm, S. Hou, Y. Lee, D. Sharp, and K. Ye. Sources of uncertainty and error in the simulation of flow in porous media. *Comp. and Applied Mathematics*, 2003. In Press. SUNYSB preprint 03-08. LANL preprint LA-UR-03-2328.
- [34] J. Glimm and H. Jin. An asymptotic analysis of two-phase fluid mixing. *Bol. Soc. Bras. Mat.*, 32:213–236, 2001.
- [35] J. Glimm, H. Jin, M. Laforest, F. Tangerman, and Y. Zhang. A two pressure numerical model of two fluid mixing. *SIAM J. Multiscale Model. Simul.*, 1:458–484, 2003.
- [36] J. Glimm, H. Jin, and Y. Zhang. Front tracking for multiphase fluid mixing. In A. A. Mammoli and C. A. Brebbia, editors, *Computational Methods in Multiphase Flow II*, pages 13–22. WIT Press, Southampton, UK, 2004.
- [37] J. Glimm, X.-L. Li, and A.-D. Lin. Nonuniform approach to terminal velocity for single mode Rayleigh-Taylor instability. *ACTA MATHEMATICAE APPLICATAE SINICA*, 18:1–8, 2002.
- [38] J. Glimm, X.-L. Li, and Y.-J. Liu. Conservative front tracking in higher space dimensions. *Transactions of Nanjing University of Aeronautics and Astronautics*, 18, Suppl.:1–15, 2001. Proceedings of International Workshop on Computational Methods for Continuum Physics and Their Applications (IWCCPA), Nanjing, China.
- [39] J. Glimm, X.-L. Li, and Y.-J. Liu. Conservative front tracking in one space dimension. *Contemporary Mathematics*, 295:253–264, 2002. Proceedings of the Joint Summer Research Conference on Fluid Flow and Transport in Porous Media: Mathematical and Numerical Treatment. In Press, Report SUNYSB-AMS-01-16.
- [40] J. Glimm, X.-L. Li, and Y.-J. Liu. Conservative front tracking with improved accuracy. *SIAM J. Numerical Analysis*, 41:1926–1947, 2003.
- [41] J. Glimm, X.-L. Li, Y.-J. Liu, and N. Zhao. Conservative front tracking and level set algorithms. *Proc. National Academy of Sci.*, 98:14198–14201, 2001.
- [42] J. Glimm, X. L. Li, W. Oh, A. Marchese, M.-N. Kim, R. Samulyak, and C. Tzanos. Jet breakup and spray formation in a diesel engine. In *Proceedings of the Second MIT Conference on Computational Fluid and Solid Mechanics*. Cambridge, MA, 2003. SUNY Stony Brook preprint No. susb-ams-02-20.
- [43] James Glimm, Yunha Lee, David H Sharp, and Kenny Q Ye. Prediction using numerical simulations, A bayesian framework for uncertainty quantification and its statistical challenge. In Bilal M. Ayyub and Nii O. Attah-Okine, editors, *Proceedings of the Fourth International Symposium on Uncertainty Modeling and Analysis (ISUMA 2003)*. IEEE, Computer Society, 2003.
- [44] H. Jin, J. Glimm, and D. H. Sharp. Two-pressure two-phase flow models. *ZAMP*, 2003. Submitted. Stony Brook University Preprint number SUNYSB-AMS-03-16 and Los Alamos National Laboratory LAUR Number LA-UR-03-7279.

- [45] H. Jin, X. F. Liu, T. Lu, B. Cheng, J. Glimm, and D. H. Sharp. Rayleigh-Taylor mixing rates for compressible flow. *Phys. Fluids*, 2004. Submitted for publication. Stony Brook University Preprint number SUNYSB-AMS-04-06 and Los Alamos National Laboratory LAUR Number LA-04-1384.
- [46] T. Lee, Y. Yu, M. Zhao, J. Glimm, X. Li, and K. Ye. Error analysis of composite shock interaction problems. *Conference Proceedings of PMC04*, 2004. (submitted) University at Stony Brook Preprint Number SB-AMS-04-08.
- [47] L. Li, J. Glimm, and X.-L. Li. All isomorphic distinct cases for multi-component interfaces in a block. *J. Comp. Appl. Mathematics*, 152:263–276, 2003.
- [48] Jee-Yeon Nam. *Linearized Analysis of the Richtmyer-Meshkov Instability for Elastic Materials*. PhD thesis, State Univ. of New York at Stony Brook, 2001.
- [49] R. Samulyak, J. Glimm, and W. Oh. A numerical algorithm for free MHD flows. *SISC (submitted)*, 2002. SUNY Stony Brook preprint.
- [50] N. Stojić, J. W. Davenport, M. Komelj, and J. Glimm. Surface magnetic moment in  $\alpha$ -uranium by density-functional theory. *Phys. Rev. B*, 68, 094407:(5 pages), 2003.
- [51] N. Stojic, J. Glimm, Y. Deng, and J. Haus. Transverse magnetic modes in two-dimensional triangular photonic crystals. *Phys. Rev. E*, 64:1–7, 2001. Paper number 056614.
- [52] J. Walter, D. Yu, B. J. Plohr, J. Grove, and J. Glimm. An algorithm for Eulerian front tracking for solid deformation. *SIAM J. Sci. Comput.*, 2003. to appear.
- [53] Y. Zhang, P. Drake, J. Glimm, J. Grove, and D. H. Sharp. Radiation coupled front tracking simulations for laser driven shock experiments. *J. Nonlinear Analysis*, 2004. Submitted. LANL report No. LA-UR-04-2381.
- [54] Wei Zhu, Xuema Wang, Yeming Ma, Manlong Rao, James Glimm, and John Kovach. Detection of cancer specific markers amidst massive mass spectral data. *Proc. Nat. Aca. Sci.*, 100:14666–14671, 2003.